

Absence of Long-Wavelength Nematic Fluctuations in LiFeAs

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Received: 12 September 2016 / Accepted: 16 September 2016 / Published online: 7 October 2016
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Abstract We investigated long-wavelength nematic fluctuations in an Fe-based superconductor LiFeAs near $\mathbf{q} = (0.05, 0, 0)$ by measuring temperature-dependent renormalization of acoustic phonons through inelastic neutron scattering. We found that the phonons have a conventional behavior, as would be expected in the absence of electronic nematic fluctuations. This observation implies that either electron-phonon coupling is too weak to see any effect or that nematic fluctuations are not present.

Keywords Pnictide · Superconductor · Nematic · INS

Just like the cuprates, iron pnictides and iron chalcogenides become superconducting when antiferromagnetic “parent” compounds are doped [1]. The parent compounds as well as low-doped superconducting ones undergo magnetic and structural phase transitions at temperatures T_N and T_S , respectively. These materials are paramagnetic and tetragonal at room temperature as a function of decreasing temperature, the system first transitions into paramagnetic orthorhombic phase below T_S and then orders antiferromagnetically below T_N with $T_N \leq T_S$. A lot of recent research

focused on the role of electronic nematicity, where electronic properties of the system occur preferentially along one of two otherwise degenerate perpendicular directions in the paramagnetic orthorhombic state [2]. A spin nematic order occurs when magnetic fluctuations break the C_4 rotational symmetry, but a magnetic order does not form [3]. Magnetoelastic coupling [4, 5] of the lattice to nematic fluctuations is responsible for orthorhombic distortion at zero and low doping. This spin-phonon coupling changes some phonon frequencies across the magnetic ordering transition, but the effect is much smaller than predicted [6, 7].

Nematic fluctuations, which are neglected in mean field approaches, have an additional effect on phonons as well as on the shear modulus C_{66} . Resonant ultrasound and 3-point bending experiments [8] showed that $\mathbf{q} = 0$ nematic fluctuations soften C_{66} . The transverse acoustic phonon branch dispersing in the $[0\ 1\ 0]$ direction that connects to the $\mathbf{q} = 0$ shear mode has the same symmetry as nematic fluctuations of the same wavevector. Therefore, buildup of these fluctuations should also soften (reduce the frequency of) these phonons.

Anomalous renormalization of these small \mathbf{q} transverse acoustic phonons was reported in Ref. [9] based on inelastic X-ray scattering measurements. More precise neutron scattering experiments demonstrated that phonons soften from about 300 K to T_N and then harden sharply following a curve reminiscent of an order parameter. This behavior relates to the previously reported anomaly in the elastic constant [10, 11] and indicates spin-phonon coupling to electronic nematic fluctuations. A quantitative study has shown that the gradual onset of the softening from far above T_N scales with the volume of correlated magnetic domains, whereas the hardening below T_N scales with the static order parameter [12]. Close correlation with magnetic properties and the similarity of the softening with the temperature dependence

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of C_{66} provided strong evidence that these phonons couple to nematic magnetic fluctuations.

In underdoped $\text{BaFe}_{2-x}\text{Co}_x\text{As}_2$ where the structural transition, T_S , appears above T_N , the phonon softening correlates with the former. Thus, the softening is directly related to the nematic phase. These underdoped samples showed an additional, entirely unexpected effect: strong phonon softening below the superconducting transition, T_c [13]. Similar measurements on optimally doped and overdoped samples where there is no structural or magnetic transition showed that the softening below T_c reflects a buildup of nematic fluctuations at nonzero wavevectors on cooling that begins far above T_c . This behavior at small nonzero wavevectors is unexpected, as nematic fluctuations at $\mathbf{q} = 0$ are suppressed by superconductivity. According to the conventional theory, this competition with superconductivity should carry over to small nonzero wavevectors, but it does not.

Here, we report neutron scattering results for a large high-quality single crystal of LiFeAs, which comes from a different (so-called 111) family of Fe-based superconductors. This material is superconducting even when it is not doped, and it remains tetragonal at all temperatures. For this work, we report \mathbf{q} , Q in reciprocal lattice units (r. l. u.), with a lattice constant of 3.77 Å.

The experiment was performed on the BT-9 MACS spectrometer at the NIST Center for Neutron Research (NCNR) using one analyzer channel. Effectively, the spectrometer was used as a cold triple-axis instrument. Measurements were performed in the vicinity of the $[2\ 0\ 0]$ Bragg peak with E_i fixed at 8 meV. A PG filter reduced higher-order neutrons. We collected good statistics at 300, 20, and 1.4 K; note that 20 K is just above the superconducting transition temperature, $T_c = 19$ K. The sample was a high-quality single crystal of LiFeAs, whose preparation is described elsewhere [14]. For the neutron measurements, we followed the experimental procedure of Ref. [10].

Figure 1 shows the results. The top panel comparing data at 300 and 20 K shows almost the same peak positions; the two peaks seem to move slightly closer together on cooling by approximately 3 %. This means that the phonon dispersion becomes steeper; i.e., there is hardening as opposed to softening observed in the 122 system. The bottom panel shows that the data at 20 and 3 K are essentially the same. In both cases, it is clear that no significant softening is occurring.

A small hardening from 300 to 20 K is expected from the conventional theory and is consistent with the reduction in the bond lengths as the lattice contracts on cooling. If nematic fluctuations build up on cooling, then softening of the phonon is expected. In this case, the peaks in Fig. 1 would move further apart. We conclude that phonons in LiFeAs do not show any signatures of nematic fluctuations,

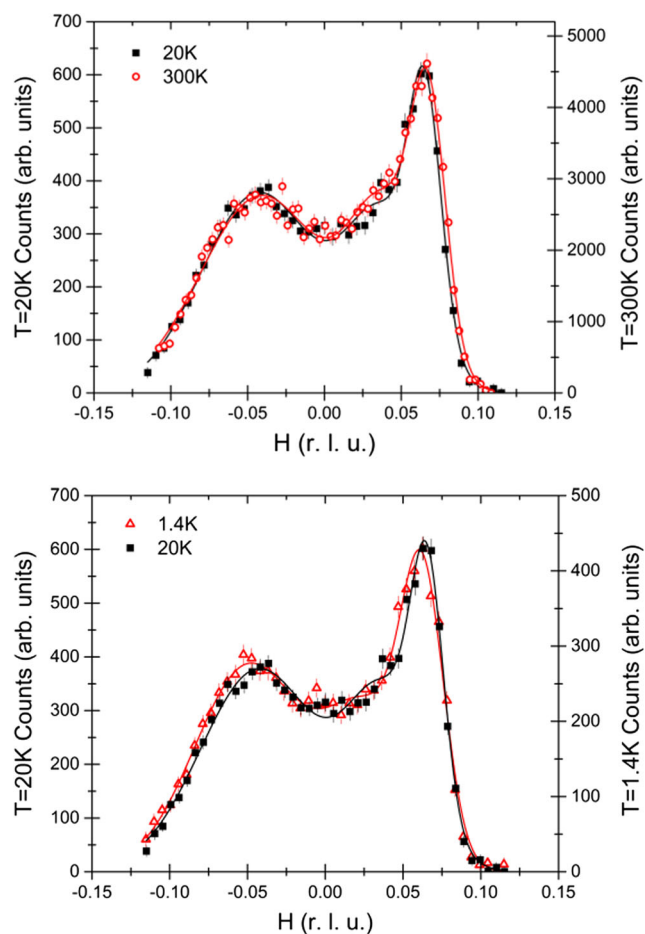


Fig. 1 Neutron scattering spectra of LiFeAs measured along $Q = (2, H, 0)$ with fixed energy transfer of 2 meV and flat background removed. The two peaks in each scan are acoustic phonons of interest discussed in the text. There is an additional contribution from longitudinal phonons centered at $h = 0$ that is picked up by the resolution function. Solid lines are guides to the eye. Error bars represent ± 1 sigma

either because the nematic fluctuations are not present or because the spin-phonon coupling is weak.

Our results are consistent with the incommensurability of magnetic fluctuations ($\delta \sim 0.07$) reported previously [15]. Furthermore, magnetic neutron scattering showed that the spectral weight of magnetic fluctuations is smaller in LiFeAs than in the 122 compounds [16]. Both of these observations can explain why nematic fluctuations in LiFeAs are not observed. It is important to perform the measurements at $\mathbf{q} = 0$ by resonant ultrasound or 3-point bending to establish the $\mathbf{q} = 0$ behavior. Based on our results, we expect that these measurements will show no signature of nematic fluctuations as well.

Acknowledgments D.R. would like to thank R. Fernandez and J. Schmalian for the helpful discussions. Y.L. would like to thank X.C. Wang for the helpful discussion about crystal growth. A.M. and D.R. were supported by the DOE, Office of Basic Energy Sciences,

Office of Science, under Contract No. DE-SC0006939. Work at Rice is supported by the DOE, BES DE-SC0012311 (P.D.), and in part by the Robert A. Welch Foundation, Grant No. C-1839 (P.D.). This work utilized the facilities supported in part by the National Science Foundation under Agreement No. DMR-1508249.

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